

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.      CIF dictionary      Interpreting this report

### Datablock: I

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Bond precision:	N- N = 0.0070 A	Wavelength=0.29521	
Cell:	a=6.819(8)	b=6.819(8)	c=9.749(9)
	alpha=90	beta=90	gamma=120
Temperature:	293 K		
	Calculated	Reported	
Volume	392.6(10)	392.6(7)	
Space group	R -3 c	R -3 c	
Hall group	-R 3 2" c	-R 3; -2" c	
Moiety formula	N4, 6(N2)	?	
Sum formula	N16	N2	
Mr	224.16	28.00	
Dx, g cm-3	2.844	2.844	
Z	3	24	
Mu (mm-1)	0.064	0.061	
F000	336.0	336.0	
F000'	335.69		
h, k, lmax	9, 9, 13	9, 9, 12	
Nref	136	79	
Tmin, Tmax		0.655, 1.000	
Tmin'			

Correction method= # Reported T Limits: Tmin=0.655 Tmax=1.000  
AbsCorr = MULTI-SCAN

Data completeness= 0.581      Theta(max)= 12.090

R(reflections)= 0.0886( 55)	wR2(reflections)=
S = 3.680	wR= 0.0803( 79)
Npar= 7	

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The following ALERTS were generated. Each ALERT has the format  
**test-name\_ALERT\_alert-type\_alert-level.**  
Click on the hyperlinks for more details of the test.

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### Alert level A

ATOM007\_ALERT\_1\_A \_atom\_site\_aniso\_label is missing  
Unique label identifying the atom site.

**Author Response: The ratio of reflections over parameters does not allow to refine the thermal parameters of the nitrogen atoms anisotropically. This is because this measurement was performed at high pressure which, due to the high pressure apparatus, limits the theta range. Indeed, the diamond anvil cell metallic body typically shadows more than 60% of the reflections.**

PLAT029\_ALERT\_3\_A \_diffrn\_measured\_fraction\_theta\_full value Low . 0.760 Why?

**Author Response: This measurement was performed at high pressure which, due to the high pressure apparatus, limits the theta range. Indeed, the diamond anvil cell metallic body typically shadows more than 60% of the reflections.**

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### Alert level C

GOODF01\_ALERT\_2\_C The least squares goodness of fit parameter lies  
outside the range 0.80 <> 2.00  
Goodness of fit given = 3.680

PLAT053_ALERT_1_C	Minimum Crystal Dimension Missing (or Error) ...	Please Check
PLAT054_ALERT_1_C	Medium Crystal Dimension Missing (or Error) ...	Please Check
PLAT055_ALERT_1_C	Maximum Crystal Dimension Missing (or Error) ...	Please Check
PLAT127_ALERT_1_C	Implicit Hall Symbol Inconsistent with Explicit -R 3;-2" c	Check
PLAT148_ALERT_3_C	s.u. on the a - Axis is (Too) Large ....	0.008 Ang.
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent .....	1 Check
	N001	
PLAT799_ALERT_4_C	Numeric Label on Displacement Par. Record .....	? Check
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.72Ang From N001 .	0.66 eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.88Ang From N001 .	-0.47 eA-3

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### Alert level G

ABSMU01\_ALERT\_1\_G Calculation of \_exptl\_absorpt\_correction\_mu  
not performed for this radiation type.

PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.125 Check
PLAT092_ALERT_4_G	Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka	0.29521 Ang.
PLAT152_ALERT_1_G	The Supplied and Calc. Volume s.u. Differ by ...	3 Units
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature ..... (K)	293 Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature ..... (K)	293 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in ..... (Resd 1 )	1.33 Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels .....	2 Note
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. #	2 Note

N2

PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT911_ALERT_3_G	Missing FCF Refl Between Thmin & STh/L= 0.600	38 Report
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	17 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF ....	2 Note
PLAT929_ALERT_5_G	No Weight Pars,Obs and Calc R1,wR2,S not Checked	! Info
PLAT966_ALERT_5_G	Note: Non-Standard (i.e. 2.0) OMIT Threshold of	3.0 Sig(I)

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2 **ALERT level A** = Most likely a serious problem - resolve or explain  
0 **ALERT level B** = A potentially serious problem, consider carefully  
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
17 **ALERT level G** = General information/check it is not something unexpected

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
5 ALERT type 3 Indicator that the structure quality may be low  
6 ALERT type 4 Improvement, methodology, query or suggestion  
4 ALERT type 5 Informative message, check

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

### Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

### Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

